Approaches for Building Stable Projection-Based Reduced Order Models

Irina Kalashnikova[1], Matthew F. Barone[2], Jeffrey A. Fike[3], Srinivasan Arunajatesan[2], Bart G. van Bloemen Waanders[4]

[1]Computational Mathematics Department, Sandia National Laboratories, Albuquerque, NM, USA.
[2]Aerosciences Department, Sandia National Laboratories, Albuquerque NM, USA.
[3]Component Science & Mechanics Department, Sandia National Laboratories, Albuquerque, NM, USA.
[4]Optimization and UQ Department, Sandia National Laboratories, Albuquerque, NM, USA.

Reduced-Order Modeling (ROM) Workshop
Livermore, CA
Thursday, August 7, 2014
SAND2014-16583PE

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Marin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94AL85000.

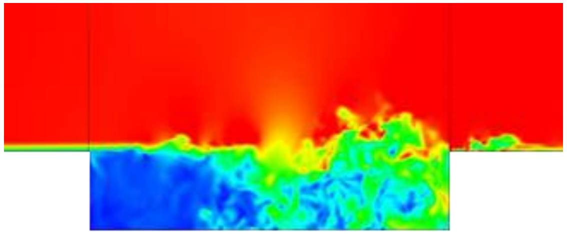
Sandia National Laboratories

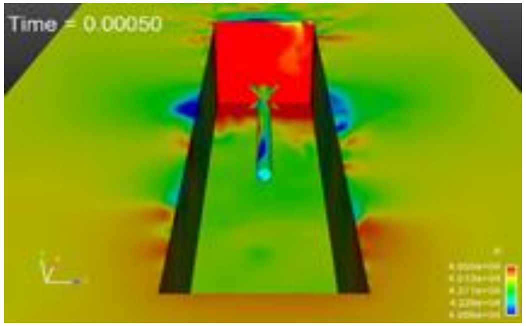
Motivation

Despite improved algorithms and powerful supercomputers, **“high-fidelity” models** are often too expensive for use in a design or analysis setting.

<u>Application areas in which this situation arises:</u>

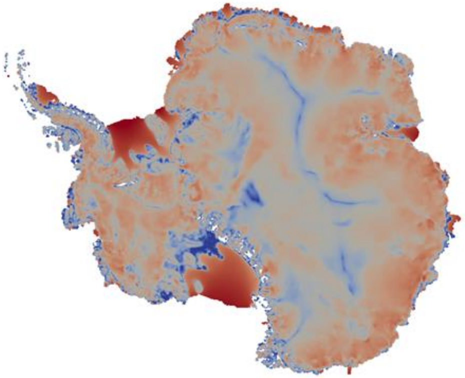
- **Compressible captive-carry** (center 1500): LES can take ***weeks*** because very fine meshes and long times are required.
- **Ice sheet modeling** (center 1400)**:** Bayesian inference of high-dimensional basal sliding field at ice bedrock is too large to solve using conventional methods (MCMC) without ROM (dimension reduction).





Antarctica Ice Sheet Example

- *Measured output*: surface velocity
- *Unknown input*: basal sliding coefficient at bedrock



Outline

- *Part 0:* Overview of POD/Galerkin Approach to Model Reduction.
- *Part 1:* Approaches for building *a priori* stable ROMs → Compressible Flow.
- *Part 2:* Approaches for stabilizing *a posteriori* unstable ROMs → Linear Time Invariant (LTI) Systems.

This work was done as a part of I. Kalashnikova's early career **LDRD** project entitled "Reduced Order Modeling for Prediction and Control of Large Scale Systems" (FY12-FY14)

[follow-up work from FY07-FY09 LDRD project led by M. Barone entitled "Reduced Order Modeling for Fluid/Structure Interaction"]

Key Research Team Members *(left to right)*: I. Kalashnikova (1442), B. van Bloemen Waanders (1441), S. Arunajatesan (1515), M. Barone (1515), J. Fike (1526)

Outline

- ***Part 0:* Overview of POD/Galerkin Approach to Model Reduction.**
- *Part 1:* Approaches for building *a priori* stable ROMs → Compressible Flow.
- *Part 2:* Approaches for stabilizing *a posteriori* unstable ROMs → Linear Time Invariant (LTI) Systems.

This work was done as a part of I. Kalashnikova’s early career **LDRD** project entitled “Reduced Order Modeling for Prediction and Control of Large Scale Systems” (FY12-FY14)

[follow-up work from FY07-FY09 LDRD project led by M. Barone entitled “Reduced Order Modeling for Fluid/Structure Interaction”]

Key Research Team Members *(left to right)*: I. Kalashnikova (1442), B. van Bloemen Waanders (1441), S. Arunajatesan (1515), M. Barone (1515), J. Fike (1526)

Proper Orthogonal Decomposition (POD)/ Galerkin Method to Model Reduction

High-Fidelity Simulations:

- Snapshot 1
- Snapshot 2
- ⋮
- Snapshot K

Step 1 →

Modal Decomposition (POD):

$$\boxed{\mathbf{x}(t) \approx \boldsymbol{\Phi}_M \mathbf{x}_M(t)}$$

Step 2 →

Galerkin Projection of LTI FOM:

$$\boxed{\boldsymbol{\Phi}_M^T \left[\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)\right]}$$

- ***Snapshot matrix***: $\boldsymbol{X} = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^K) \in \mathbb{R}^{NxK}$
- ***SVD:*** $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$
- ***Truncation:*** $\boldsymbol{\Phi}_M = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_M) = \boldsymbol{U}(:, 1{:}M)$

N = # of dofs in high-fidelity simulation
K = # of snapshots
M = # of dofs in ROM
($M << N, M << K$)

"Small" ROM LTI System:

$$\boxed{\begin{array}{rcl} \dot{\mathbf{x}}_M(t) & = & \boldsymbol{\Phi}_M^T \mathbf{A} \boldsymbol{\Phi}_M \mathbf{x}_M(t) + \boldsymbol{\Phi}_M^T \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}_M(t) & = & \mathbf{C}\boldsymbol{\Phi}_M \mathbf{x}_M(t) \end{array}}$$

Continuous vs. Discrete Galerkin Projection

Continuous Projection

Governing PDEs
$\dot{\boldsymbol{q}} = \mathcal{L}\boldsymbol{q}$

↓

High-fidelity model
$\dot{\boldsymbol{q}}_N = \boldsymbol{A}_N \boldsymbol{q}_N$

↓

Continuous modal basis* $\boldsymbol{\phi}_j(\boldsymbol{x})$

↓

Projection of governing PDEs (numerical integration)

↓

ROM
$\dot{a}_j = (\boldsymbol{\phi}_j, \mathcal{L}\boldsymbol{\phi}_k) a_k$

If PDEs are linear or have polynomial non-linearities, projection can be calculated in **offline stage** of MOR.

Part 1 of talk.

Part 2 of talk.

Discrete Projection

Governing PDEs
$\dot{\boldsymbol{q}} = \mathcal{L}\boldsymbol{q}$

↓

High-fidelity model
$\dot{\boldsymbol{q}}_N = \boldsymbol{A}_N \boldsymbol{q}_N$

↓

Discrete modal basis $\boldsymbol{\Phi}$

↓

Projection of HF model (matrix operation)

↓

ROM
$\dot{\boldsymbol{a}}_M = \boldsymbol{\Phi}^T \boldsymbol{A}_N \boldsymbol{\Phi} \boldsymbol{a}_M$

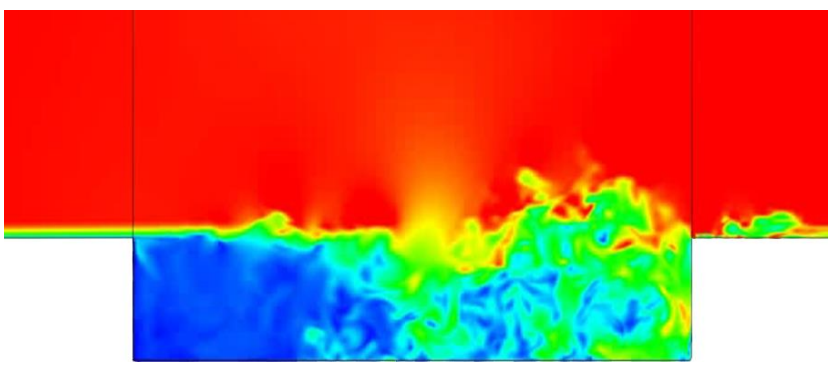
* Continuous functions space is defined using finite elements.

Stability Issues of POD/Galerkin ROMs

Full Order Model (FOM)	**Reduced Order Model (ROM)**
$\dot{\boldsymbol{q}}(t) = \mathcal{L}\boldsymbol{q}(t) + \mathcal{N}(\boldsymbol{q}(t))$	$\dot{\boldsymbol{q}}_M(t) = \boldsymbol{A}_M\boldsymbol{q}_M(t) + \boldsymbol{N}_M(\boldsymbol{q}_M(t))$

Problem: FOM stable $\not\Rightarrow$ ROM stable!

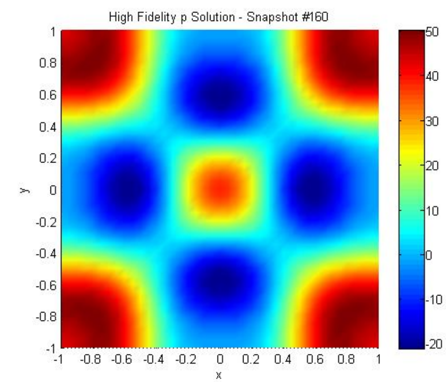
- There is no *a priori* stability guarantee for POD/Galerkin ROMs.
- Stability of a ROM is commonly evaluated *a posteriori* – **RISKY!**
- Instability of POD/Galerkin ROMs is a **real** problem in some applications…

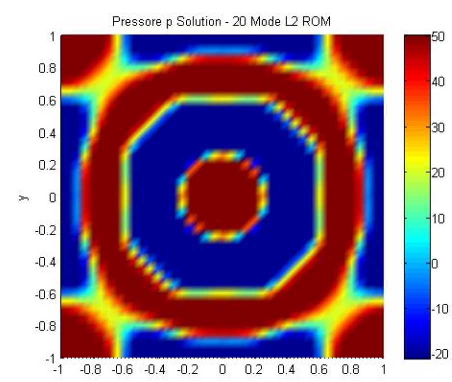


…e.g., compressible flows, high-Reynolds number flows.

Top right: FOM

Bottom right: ROM





LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Outline

- *Part 0:* Overview of POD/Galerkin Approach to Model Reduction.
- ***Part 1:* Approaches for building *a priori* stable ROMs → Compressible Flow.**
- *Part 2:* Approaches for stabilizing *a posteriori* unstable ROMs → Linear Time Invariant (LTI) Systems.

This work was done as a part of I. Kalashnikova's early career **LDRD** project entitled "Reduced Order Modeling for Prediction and Control of Large Scale Systems" (FY12-FY14)

[follow-up work from FY07-FY09 LDRD project led by M. Barone entitled "Reduced Order Modeling for Fluid/Structure Interaction"]

***Key Research Team Members** (left to right)*: I. Kalashnikova (1442), B. van Bloemen Waanders (1441), S. Arunajatesan (1515), M. Barone (1515), J. Fike (1526)

Energy-Stability

- **Practical Definition:** Numerical solution does not “blow up” in finite time.
- **More Precise Definition:** Numerical discretization does not introduce any spurious instabilities inconsistent with natural instability modes supported by the governing continuous PDEs.

Numerical solutions must maintain proper **energy balance**.

- Stability of ROM is intimately tied to choice of **inner product** for the Galerkin projection.
- Stability-preserving inner product derived using the **energy method**:
    - Bounds numerical solution energy in a physical way.
    - Borrowed from spectral methods community.
    - Analysis is straightforward for ROMs constructed via **continuous projection.**

Practical implication of energy-stability analysis:
energy inner product ensures that any “bad” modes will not introduce spurious non-physical numerical instabilities into the Galerkin approximation.

Linearized Compressible Flow Equations

Energy-Stability for Linearized PDEs:
FOM linearly stable ⇒ ROM built in energy inner product linearly stable ($Re(\lambda) < 0$)
(Barone *et al.* 2009, Kalashnikova *et al.* 2012)

Linearized compressible Euler/Navier-Stokes equations are appropriate when a compressible fluid system can be described by small-amplitude perturbations about a steady-state mean flow.

- Linearization of full compressible Euler/Navier-Stokes equations obtained as follows:
  1. Decompose fluid field as **steady mean** plus **unsteady fluctuation**

$$\boldsymbol{q}(\boldsymbol{x},t) = \overline{\boldsymbol{q}}(\boldsymbol{x}) + \boldsymbol{q}'(\boldsymbol{x},t)$$

  2. Linearize full nonlinear compressible Navier-Stokes equations around steady mean to yield **linear hyperbolic/incompletely parabolic** system

$$\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\boldsymbol{K}_{ij}(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial x_i}\right] = \boldsymbol{0}$$

Sandia National Laboratories

Energy-Stable ROMs for Linearized Compressible Flow

Linearized compressible Euler/Navier-Stokes equations are **symmetrizable** (Barone & Kalashnikova, 2009; Kalashnikova & Arunajatesan, 2012).

- There exists a symmetric positive definite matrix $\boldsymbol{H} \equiv \boldsymbol{H}(\overline{\boldsymbol{q}})$ (system "**symmetrizer**") s.t.:
  - The convective flux matrices $\boldsymbol{H}\boldsymbol{A}_i$ are symmetric
  - The following augmented viscosity matrix is symmetric positive semi-definite

$$\boldsymbol{K}^s = \begin{pmatrix} \boldsymbol{H}\boldsymbol{K}_{11} & \boldsymbol{H}\boldsymbol{K}_{12} & \boldsymbol{H}\boldsymbol{K}_{13} \\ \boldsymbol{H}\boldsymbol{K}_{21} & \boldsymbol{H}\boldsymbol{K}_{22} & \boldsymbol{H}\boldsymbol{K}_{23} \\ \boldsymbol{H}\boldsymbol{K}_{31} & \boldsymbol{H}\boldsymbol{K}_{32} & \boldsymbol{H}\boldsymbol{K}_{33} \end{pmatrix}$$

Symmetry Inner Product (weighted L^2 inner product):

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{\boldsymbol{H}} = \int_{\Omega} \boldsymbol{q}_1 \boldsymbol{H} \boldsymbol{q}_2 d\Omega$$

- If ROM is built in **symmetry inner product**, Galerkin approximation will satisfy the same energy expression as continuous PDEs:

$$\left|\left|\boldsymbol{q}'_M(\boldsymbol{x},t)\right|\right|_{\boldsymbol{H}} \leq e^{\beta t} \left|\left|\boldsymbol{q}'_M(\boldsymbol{x},0)\right|\right|_{\boldsymbol{H}} \quad \left(\Rightarrow \frac{dE_M}{dt} \leq 0 \text{ for uniform base flow}\right)$$

Sandia National Laboratories

Symmetrizers for Several Hyperbolic/ Incompletely Parabolic Systems

- ***Wave equation:*** $\ddot{u} = a^2 \frac{\partial^2 u}{\partial x^2}$ or $\dot{\boldsymbol{q}} = \boldsymbol{A} \frac{\partial \boldsymbol{q}}{\partial x}$ where $\boldsymbol{q} = \left(\dot{u}, \frac{\partial u}{\partial x}\right)$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} 1 & 0 \\ 0 & a^2 \end{pmatrix}$

- ***Linearized shallow water equations:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}}) \frac{\partial \boldsymbol{q}'}{\partial x_i} = \boldsymbol{0}$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\phi} & 0 & 0 \\ 0 & \bar{\phi} & 0 \\ 0 & 0 & 1 \end{pmatrix}$

- ***Linearized compressible Euler:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}}) \frac{\partial \boldsymbol{q}'}{\partial x_i} = \boldsymbol{0}$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\rho} & 0 & 0 \\ 0 & \alpha^2 \gamma \bar{\rho}^2 \bar{p} & \bar{\rho}\alpha^2 \\ 0 & 0 & \frac{(1+\alpha^2)}{\gamma \bar{p}} \end{pmatrix}$

- ***Linearized compressible Navier-Stokes:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}}) \frac{\partial \boldsymbol{q}'}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\boldsymbol{K}_{ij}(\overline{\boldsymbol{q}}) \frac{\partial \boldsymbol{q}'}{\partial x_i}\right] = \boldsymbol{0}$

$$\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\rho} & 0 & 0 \\ 0 & \frac{\bar{\rho} R}{\overline{\overline{T}(\gamma - 1)}} & 0 \\ 0 & 0 & \frac{R\overline{T}}{\bar{\rho}} \end{pmatrix}$$

- Barone & Kalashnikova, *JCP*, 2009.
- Kalashnikova & Arunajatesan, *WCCM X*, 2012.
- Kalashnikova *et al.*, *SAND report*, 2014.

Sandia National Laboratories

Continuous Projection Implementation: "Spirit" Code

"Spirit" ROM Code = 3D parallel C++ POD/Galerkin test-bed ROM code that uses data-structures and eigensolvers from **Trilinos** to build energy-stable ROMs for compressible flow problems → stand-alone code that can be synchronized with any high-fidelity code!

- POD modes defined using piecewise smooth finite elements.
- Gauss quadrature rules of sufficient accuracy are used to compute exactly inner products with the help of the `libmesh` library.
- Physics in Spirit:
  - ***Linearized compressible Euler*** (L^2, energy inner product).
  - ***Linearized compressible Navier-Stokes*** (L^2, energy inner product).
  - ***Nonlinear isentropic compressible Navier-Stokes*** (L^2, stagnation energy, stagnation enthalpy inner product).
  - ***Nonlinear compressible Navier-Stokes*** (L^2, energy inner product).

First, testing of ROMs for these physics

"SIGMA CFD" High-Fidelity Code = Sandia in-house finite volume flow solver derived from LESLIE3D (Genin & Menon, 2010), an LES flow solver originally developed in the Computational Combustion Laboratory at Georgia Tech.

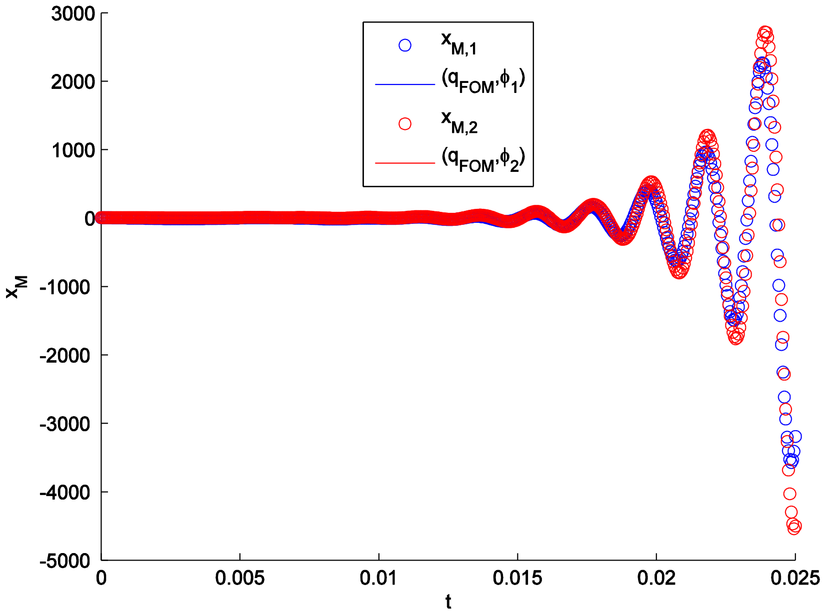
Sandia National Laboratories

Numerical Experiment: 2D Inviscid Pressure Pulse

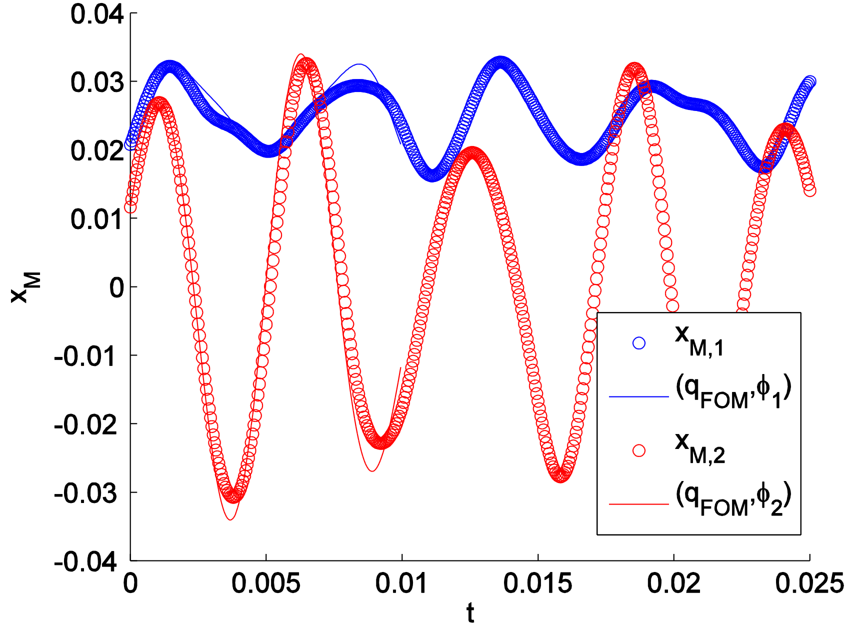
- Inviscid pulse in a uniform base flow (linear dynamics).
- High-fidelity simulation run on mesh with 3362 nodes, up to time $t = 0.01$ seconds.
- 200 snapshots of solution used to construct $M = 20$ mode ROM in L^2 and symmetry inner products.

$x_{M,i}(t)$ vs. $(\boldsymbol{q}'_{CFD}, \boldsymbol{\phi}_i)$ for $i = 1{,}2$

L^2 ROM



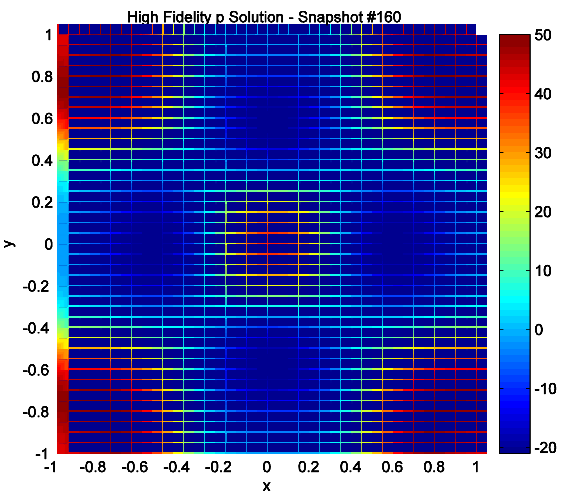
Symmetry ROM



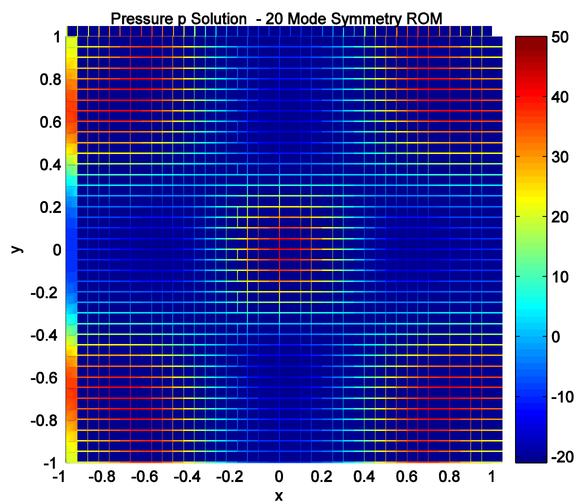
Numerical Experiment: 2D Inviscid Pressure Pulse (cont’d)

- Inviscid pulse in a uniform base flow (linear dynamics).
- High-fidelity simulation run on mesh with 3362 nodes, up to time $t = 0.01$ seconds.
- 200 snapshots of solution used to construct $M = 20$ mode ROM in L^2 and symmetry inner products.

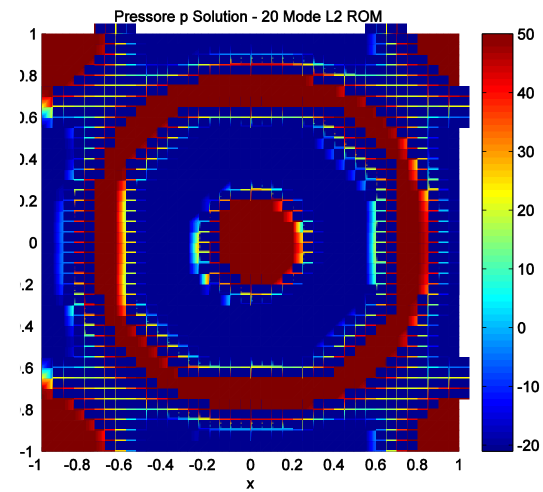
p’: High-fidelity



p’: Symmetry ROM



p’: L^2 ROM



time of snapshot 160

Nonlinear Compressible Flow Equations

Energy-Stability for Nonlinear PDEs:
ROM built in energy inner product will preserve stability of an equilibrium point at 0 for the governing nonlinear system of PDEs (Rowley, 2004; Kalashnikova *et al., 2014*).

- Compressible isentropic Navier-Stokes equations (cold flows, moderate Mach #):

$$\frac{Dh}{Dt} + (\gamma - 1)h\nabla \cdot \boldsymbol{u} = 0$$
$$\frac{D\boldsymbol{u}}{Dt} + \nabla h - \frac{1}{Re}\Delta\boldsymbol{u} = \boldsymbol{0}$$

h = enthalpy
$\boldsymbol{u}$ = velocity vector
ρ = density
T = temperature
$\boldsymbol{\tau}$ = viscous stress tensor

- Full compressible Navier-Stokes equations:

$$\rho\frac{D\boldsymbol{u}}{Dt} + \frac{1}{\gamma M^2}\nabla(\rho T) - \frac{1}{Re}\nabla \cdot \boldsymbol{\tau} = \boldsymbol{0}$$
$$\frac{D\rho}{Dt} + \rho\nabla \cdot \boldsymbol{u} = 0$$
$$\rho\frac{DT}{Dt} + (\gamma - 1)\rho T\nabla \cdot \boldsymbol{u} - \frac{\gamma}{PrRe}\nabla \cdot (\kappa\nabla T) - \left(\frac{\gamma(\gamma-1)M^2}{Re}\right)\nabla\boldsymbol{u} \cdot \boldsymbol{\tau} = 0$$

Energy-Stable ROMs for Nonlinear Compressible Flow (Isentropic NS)

In (Rowley, 2004), Rowley *et al.* showed that energy inner product for the compressible isentropic Navier-Stokes equations can be defined following a transformation of these equations.

- Transformed compressible isentropic Navier-Stokes equations:

$$\begin{aligned} \frac{Dc}{Dt} + \frac{\gamma-1}{2} c \nabla \cdot \boldsymbol{u} \qquad\qquad &= 0 \\ \frac{D\boldsymbol{u}}{Dt} + \frac{2}{\gamma-1} c \nabla c - \frac{1}{Re} \Delta \boldsymbol{u} &= \boldsymbol{0} \end{aligned}$$

c = speed of sound ($c^2 = (\gamma - 1)h$)
$\boldsymbol{u}$ = velocity

- Family of inner products:

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_\alpha = \int_\Omega \left(\boldsymbol{u}_1 \cdot \boldsymbol{u}_2 + \frac{2\alpha}{\gamma - 1} c_1 c_2 \right) d\Omega$$

$$\alpha = \begin{cases} 1 \Rightarrow ||\boldsymbol{q}||_\alpha = \text{stagnation enthalpy} \\ \frac{1}{\gamma} \Rightarrow ||\boldsymbol{q}||_\alpha = \text{stagnation energy} \end{cases}$$

If Galerkin projection step of model reduction is performed in α inner product, then the Galerkin projection will **preserve the stability of an equilibrium point at the origin** (Rowley, 2004).

Energy-Stable ROMs for Nonlinear Compressible Flow (Full NS)

Our recent work extends ideas in (Rowley, 2004) to **full compressible N-S equations**.
Requirement: *transformation/inner product yields PDEs with only polynomial non-linearities.*

- First, full compressible Navier-Stokes equations are **transformed** into the following variables:

$$a = \sqrt{\rho}, \quad \boldsymbol{b} = a\boldsymbol{u}, \; d = ae$$

e =internal energy

- Next, the following **"total energy"** inner product is defined:

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{TE} = \int_\Omega (\boldsymbol{b}_1 \cdot \boldsymbol{b}_2 + a_1 d_2 + a_2 d_1) d\Omega$$

→ Norm induced by total energy inner product is the total energy of the fluid system:

$$\boxed{||\boldsymbol{q}||_{TE} = \int_\Omega \left(\rho e + \frac{1}{2}\rho u_i u_i\right) d\Omega}$$

If Galerkin projection step of model reduction is performed in total energy inner product, then the Galerkin projection will **preserve the stability of an equilibrium point at the origin** (Kalashnikova *et al.*, 2014)

☺ Transformed equations have only **polynomial non-linearities** (projection of which can be computed in offline stage of MOR and stored).

☹ Transformation introduces **higher order polynomial** non-linearities for viscous case.

☺ Efficiency of online stage of MOR can be recovered using **interpolation** (e.g., DEIM, gappy POD).

Sandia National Laboratories

Continuous Projection Implementation: "Spirit" Code

"Spirit" ROM Code = 3D parallel C++ POD/Galerkin test-bed ROM code that uses data-structures and eigensolvers from **Trilinos** to build energy-stable ROMs for compressible flow problems → stand-alone code that can be synchronized with any high-fidelity code!

- POD modes defined using piecewise smooth finite elements.
- Gauss quadrature rules of sufficient accuracy are used to compute exactly inner products with the help of the libmesh library.
- Physics in spirit:
  - ***Linearized compressible Euler*** (L^2, energy inner product).
  - ***Linearized compressible Navier-Stokes*** (L^2, energy inner product).
  - ***Nonlinear isentropic compressible Navier-Stokes*** (L^2, stagnation energy, stagnation enthalpy inner product).
  - ***Nonlinear compressible Navier-Stokes*** (L^2, energy inner product).

Now, testing of ROMs for these physics

"SIGMA CFD" High-Fidelity Code = Sandia in-house finite volume flow solver derived from LESLIE3D (Genin & Menon, 2010), a LES flow solver originally developed in the Computational Combustion Laboratory at Georgia Tech.

Sandia National Laboratories

Numerical Experiment: Viscous Laminar Cavity

- Viscous cavity problem at $M = 0.6$, $Re = 1500$ (laminar regime).

- **High-fidelity simulation**: DNS based on full nonlinear compressible Navier-Stokes equations with 99,408 nodes (right).

- 500 snapshots collected, every $\Delta t_{snap} = 1 \times 10^{-4}$ seconds.

- Snapshots used to construct $M = 5$ mode ROM for nonlinear compressible Navier-Stokes equations in $\boldsymbol{L^2}$ **and total energy inner products**.

- $M = 5$ mode POD bases capture $\approx$ 99% of snapshot energy.

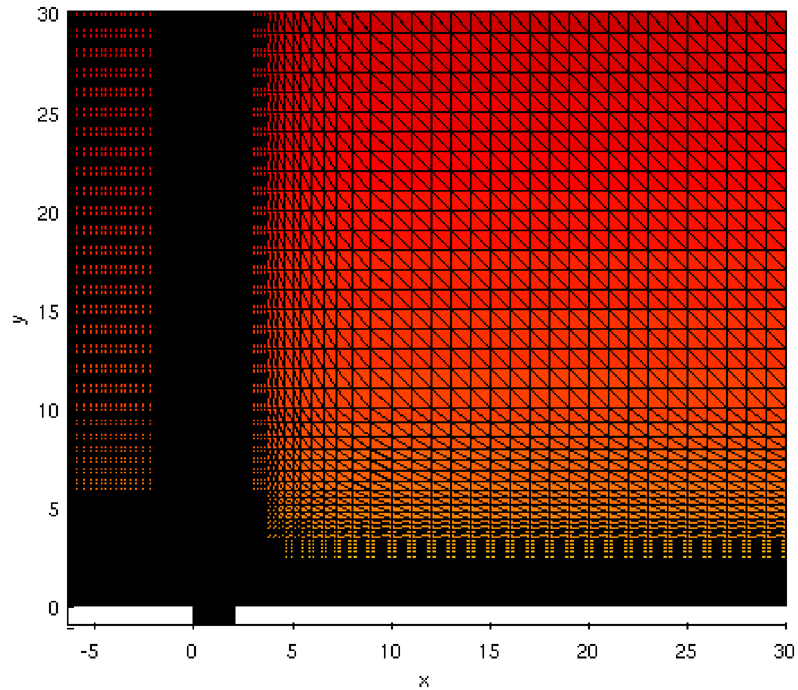


Figure above: viscous laminar cavity problem domain/mesh.

Numerical Experiment: Viscous Laminar Cavity (cont'd)

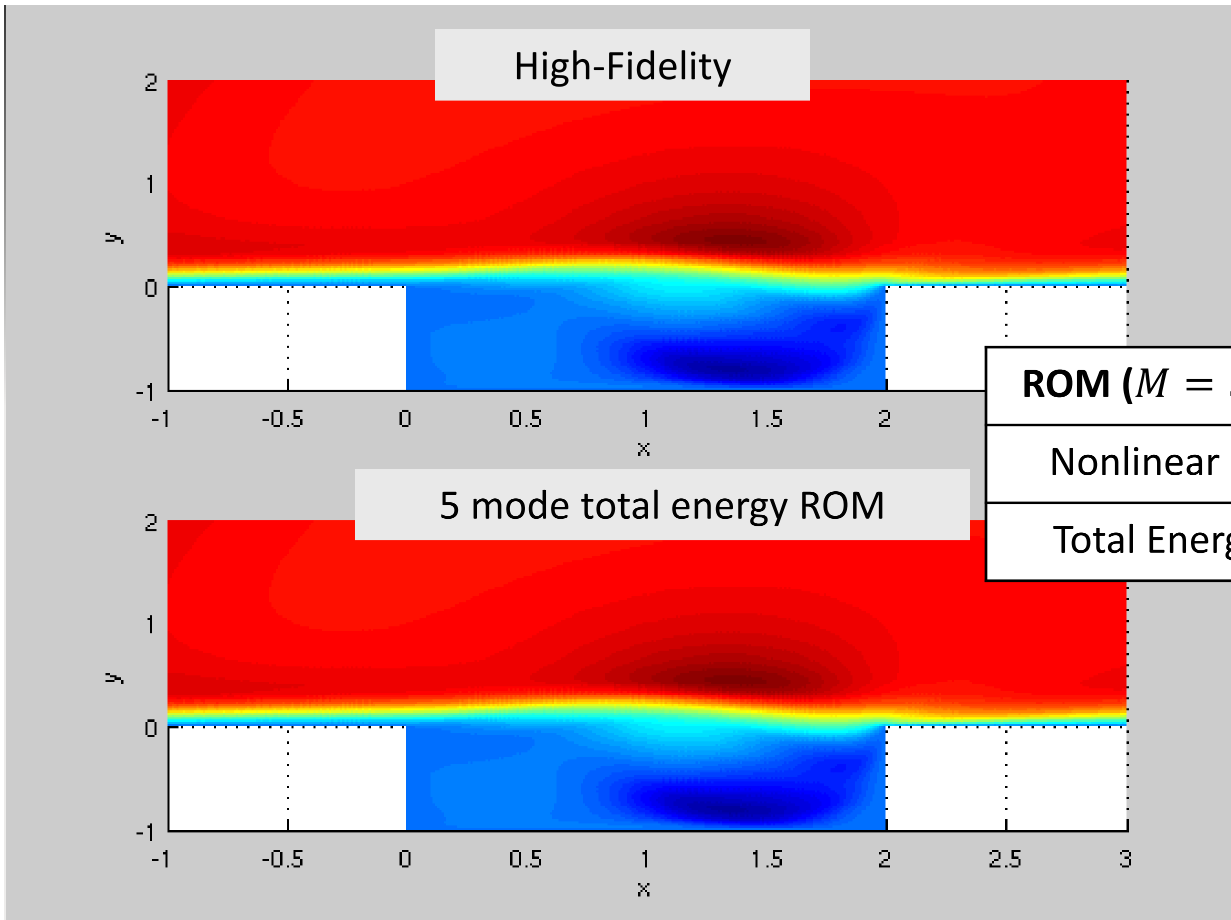


Figure above: u-component of velocity as a function of time t

- **Ongoing work:** understanding effects of boundary conditions on ROM stability/accuracy.

ROM ($M = 5$ modes)	Error (L^2 norm)
Nonlinear L^2 ROM	NaN
Total Energy ROM	5.52×10^{-2}

- **Future work:** improving efficiency of total energy ROMs through incorporation of interpolation (e.g., DEIM, gappy POD).

Outline

- *Part 0:* Overview of POD/Galerkin Approach to Model Reduction.
- *Part 1:* Approaches for building *a priori* stable ROMs → Compressible Flow.
- ***Part 2:* Approaches for stabilizing *a posteriori* unstable ROMs → Linear Time Invariant (LTI) Systems.**

This work was done as a part of I. Kalashnikova's early career **LDRD** project entitled "Reduced Order Modeling for Prediction and Control of Large Scale Systems" (FY12-FY14)

[follow-up work from FY07-FY09 LDRD project led by M. Barone entitled "Reduced Order Modeling for Fluid/Structure Interaction"]

***Key Research Team Members** (left to right)*: I. Kalashnikova (1442), B. van Bloemen Waanders (1441), S. Arunajatesan (1515), M. Barone (1515), J. Fike (1526)

Stable ROMs for Linear Time Invariant Systems

Attention restricted to **Linear Time Invariant (LTI) systems**

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t)$$
$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t)$$

as a first step towards the more general nonlinear case.

LTI Full Order Model (FOM)

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t)$$
$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t)$$

LTI Reduced Order Model (ROM)

$$\dot{\boldsymbol{x}}_M(t) = \boldsymbol{A}_M\boldsymbol{x}_M(t) + \boldsymbol{B}_M\boldsymbol{u}(t)$$
$$\boldsymbol{y}_M(t) = \boldsymbol{C}_M\boldsymbol{x}_M(t)$$

Problem: $\boldsymbol{A}$ stable $\not\Rightarrow$ $\boldsymbol{A}_M$ stable!

Solution:

Unstable ROM ($\boldsymbol{A}_M$ unstable) → Black box: Stabilization Algorithm ($\boldsymbol{A}_M \leftarrow \widetilde{\boldsymbol{A}}_M$) → Stable and Accurate ROM ($\widetilde{\boldsymbol{A}}_M$ stable)

ROM Stabilization via Optimization-Based Eigenvalue Reassignment

ROM Stabilization Optimization Problem
(Constrained Nonlinear Least Squares):

$$\min_{\lambda_i^u} \sum_{k=1}^{K} ||\boldsymbol{y}^k - \boldsymbol{y}_M{}^k||_2{}^2 \qquad (1)$$
$$s.t.\ Re(\lambda_i{}^u) < 0$$

Idea: modify ROM system s.t. $\boldsymbol{A}_M$ is stable and discrepancy b/w ROM output $\boldsymbol{y}_M(t)$ and FOM output $\boldsymbol{y}(t)$ is minimal.

Replace unstable $\boldsymbol{A}_M$ with stable $\widetilde{\boldsymbol{A}}_M$.

- $\lambda_i{}^u$ = unstable eigenvalues of original ROM matrix $\boldsymbol{A}_M$.
- $\boldsymbol{y}^k = \boldsymbol{y}(t_k) =$ snapshot output at t_k.
- $\boldsymbol{y}_M{}^k = \boldsymbol{C}_M \left[\exp(t_k \boldsymbol{A}_M)\, \boldsymbol{x}_M(0) + \int_0^{t_k} \exp\{(t_k - \tau)\, \boldsymbol{A}_M\} \boldsymbol{B}_M u(\tau) d\tau\right]$ = ROM output at t_k.
- ROM stabilization optimization problem is small: $< O(M)$.
- ROM stabilization optimization problem can be solved by standard optimization algorithms, e.g., interior point method.
  - We use `fmincon` function in MATLAB's optimization toolbox.
  - We implement ROM stabilization optimization problem in ***characteristic variables*** $\boldsymbol{z}_M(t) = \boldsymbol{S}_M{}^{-1}\boldsymbol{x}_M(t)$ where $\boldsymbol{A}_M = \boldsymbol{S}_M \boldsymbol{D}_M \boldsymbol{S}_M{}^{-1}$.

ROM Stabilization via Optimization-Based Eigenvalue Reassignment (cont'd)

Algorithm

- Diagonalize the ROM matrix $\boldsymbol{A}_M$: $\boldsymbol{A}_M = \boldsymbol{S}_M \boldsymbol{D}_M \boldsymbol{S}_M^{-1}$.
- Initialize a diagonal $M \times M$ matrix $\widetilde{\boldsymbol{D}}_M$. Set $j = 1$.
- **for** $i = 1$ to M
    - **if** $Re(D_M(i,i) < 0)$, set $\widetilde{D}_M(i,i) = D_M(i,i)$.
    - **else**, set $\widetilde{D}_M(i,i) = \lambda_j^u$.
- Increment $j \leftarrow j + 1$.
- Solve the optimization problem (1) for the eigenvalues $\{\lambda_j^u\}$ using an optimization algorithm (e.g., interior point method).
- Evaluate $\widetilde{\boldsymbol{D}}_M$ at the solution of the optimization problem (1).
- Return the stabilized ROM system, given by $\boldsymbol{A}_M \leftarrow \widetilde{\boldsymbol{A}}_M = \boldsymbol{S}_M \widetilde{\boldsymbol{D}}_M \boldsymbol{S}_M^{-1}$.

- Solution to optimization problem (1) may not be unique.
- Can solve (1) for real or complex-conjugate pair eigenvalues:
    - $\lambda_j^u \in \mathbb{R}$ s.t. constraint $\lambda_j^u < 0$.
    - $\lambda_j^u = \lambda_j^{ur} + i\,\lambda_j^{uc}$, $\lambda_{j+1}^u = \lambda_j^{ur} - i\,\lambda_j^{uc} \in \mathbb{C}$ where $\lambda_j^{ur}, \lambda_j^{uc} \in \mathbb{R}$ s.t. constraint $\lambda_j^{ur} < 0$.

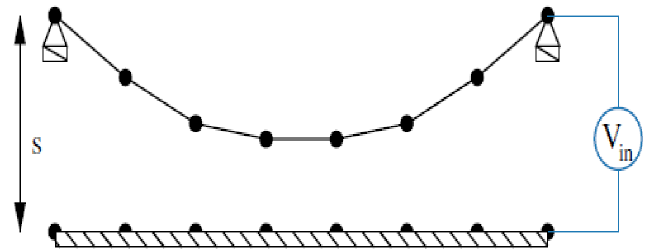
Sandia National Laboratories

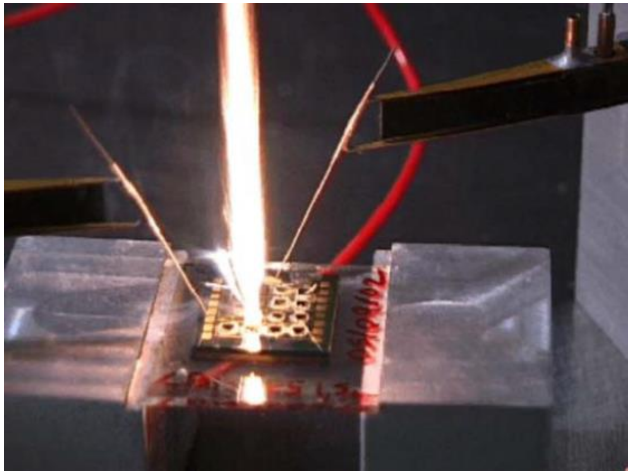
Numerical Results: Electrostatically Actuated Beam Benchmark

- FOM = 1D model of electrostatically actuated beam.
- Application of model: microelectromechanical systems (MEMS) devices such as electromechanical radio frequency (RF) filters.
- 1 input corresponding to periodic on/off switching, 1 output, initial condition $\boldsymbol{x}(0) = \mathbf{0}_N$.
- Second order linear semi-discrete system of the form:

$$\boldsymbol{M}\ddot{\boldsymbol{x}}(t) + \boldsymbol{E}\dot{\boldsymbol{x}}(t) + \boldsymbol{K}\boldsymbol{x}(t) = \boldsymbol{B}\boldsymbol{u}(t)$$
$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t)$$

- Matrices $\boldsymbol{M}, \boldsymbol{E}, \boldsymbol{K}, \boldsymbol{B}, \boldsymbol{C}$ specifying the problem downloaded from the Oberwolfach ROM repository*.
- 2nd order linear system re-written as 1st order LTI system for purpose of analysis/model reduction.





- FOM is stable.

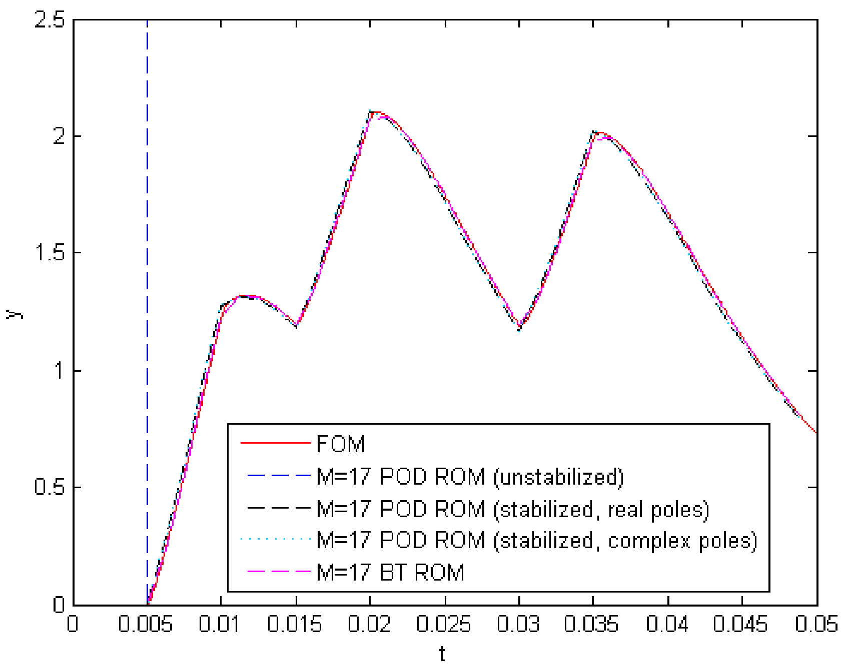
* Oberwolfach ROM benchmark repository: http://simulation.uni-freiburg.de/downloads/benchmark.

Numerical Results #2: Electrostatically Actuated Beam Benchmark (cont'd)

- $M = 17$ POD/Galerkin ROM constructed from $K = 1000$ snapshots up to time $t = 0.05$.
- $M = 17$ POD/Galerkin ROM has 4 unstable eigenvalues (all real).
  - Two options for ROM stabilization optimization problem:

    Option 1: Solve for $\lambda_1, \lambda_2, \lambda_3, \lambda_4 \in \mathbb{R}$ s.t. the constraint $\lambda_1, \lambda_2, \lambda_3, \lambda_4 < 0$.

    Option 2: Solve for $\lambda_1 + \lambda_2 i, \lambda_1 - \lambda_2 i, \lambda_3 + \lambda_4 i, \lambda_3 - \lambda_4 i \in \mathbb{C}$ s.t. the constraint $\lambda_1, \lambda_3 < 0$.
- Initial guess for $\texttt{fmincon}$ interior point method: $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = -1$.



ROM	$\frac{\sqrt{\sum_{k=1}^{K} \|\|\boldsymbol{y}^k - \boldsymbol{y}_M{}^k\|\|_2{}^2}}{\sqrt{\sum_{k=1}^{K} \|\|\boldsymbol{y}_k\|\|_2{}^2}}$
Unstabilized POD	NaN
Optimization Stabilized POD (Real Poles)	0.0194
Optimization Stabilized POD (Complex-Conjugate Poles)	0.0205
Balanced Truncation	$1.370e-6$

Sandia National Laboratories

Summary & Future Work

<u>Part 1:</u> Approaches for building *a priori* stable ROMs (for Compressible Flow using Continuous Projection)

- It is shown that the choice of inner product for the Galerkin projection step is crucial to stability of the ROM.
  - For ***linearized compressible flow***, Galerkin projection in the “symmetry” inner product leads to a ROM that is energy-stable for any choice of basis.
  - For ***nonlinear compressible flow***, an inner product that induces the total energy of the fluid system is developed. A ROM constructed in this inner product will preserve the stability of an equilibrium point at 0 for the system.
- ***Ongoing/future work:*** improving efficiency of total energy ROMs through interpolation (e.g., DEIM, gappy POD); incorporating BCs into Spirit code.

<u>Part 2:</u> Approaches for stabilizing *a posteriori* unstable ROMs (for Linear Time Invariant, or LTI, Systems).

- A ***new*** ROM stabilization approach that modifies *a posteriori* an unstable ROM LTI system by changing the system’s unstable eigenvalues is proposed.
- In the proposed stabilization algorithm, a constrained nonlinear least squares optimization problem for the ROM eigenvalues is formulated to minimize error in ROM output.
- ***Future work:*** extension to nonlinear problems and predictive applications.

Acknowledgements

This work was funded by the Laboratories' Directed Research and Development (**LDRD**) Program at **Sandia National Laboratories**.

Special thanks to: Prof. Lou Cattafesta (FSU) and Prof. Karen Willcox (MIT) for useful discussions that led to some of the ideas presented in Part 2 of the talk.

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Thank You! Questions?

ikalash@sandia.gov

http://www.sandia.gov/~ikalash

Sandia National Laboratories

Some references on these ideas:

- **I. Kalashnikova**, S. Arunajatesan, M.F. Barone, B.G. van Bloemen Waanders, J.A. Fike. Reduced Order Modeling for Prediction and Control of Large-Scale Systems. *Sandia National Laboratories Report, SAND No. 2014-4693* (2014).
- **I. Kalashnikova**, B.G. van Bloemen Waanders, S. Arunajatesan, M.F. Barone. "Stabilization of Projection-Based Reduced Order Models for Linear Time-Invariant Systems via Optimization-Based Eigenvalue Reassignment". *Comput. Meth. Appl. Mech. Engng.* **272** (2014) 251-270.
- M.F. Barone, **I. Kalashnikova**, D.J. Segalman, H. Thornquist. Stable Galerkin reduced order models for linearized compressible flow. *J. Comput. Phys.* ***288:*** 1932-1946, 2009.

References

- **I. Kalashnikova**, B.G. van Bloemen Waanders, S. Arunajatesan, M.F. Barone. "Stabilization of Projection-Based Reduced Order Models for Linear Time-Invariant Systems via Optimization-Based Eigenvalue Reassignment". *Comput. Meth. Appl. Mech. Engng.* **272** (2014) 251-270.
- M.F. Barone, **I. Kalashnikova**, D.J. Segalman, H. Thornquist. Stable Galerkin reduced order models for linearized compressible flow. *J. Comput. Phys.* **288:** 1932-1946, 2009.
- C.W. Rowley, T. Colonius, R.M. Murray. Model reduction for compressible flows using POD and Galerkin projection. *Physica D.* **189**: 115-129, 2004.
- G. Serre, P. Lafon, X. Gloerfelt, C. Bailly. Reliable reduced-order models for time-dependent linearized Euler equations. *J. Comput. Phys.* **231**(15): 5176-5194, 2012.
- B. Bond, L. Daniel, Guaranteed stable projection-based model reduction for indefinite and unstable linear systems, In: *Proceedings of the 2008 IEEE/ACM International Conference on Computer-Aided Design*, 728–735, 2008.
- D. Amsallem, C. Farhat. Stabilization of projection-based reduced order models. *Int. J. Numer. Methods Engng.* **91** (4) (2012) 358-377.
- F. Genin and S. Menon. Studies of shock/turbulent shear layer interaction using large-eddy simulation. *Computers and Fluids,* **39** 800–819 (2010).

- **I. Kalashnikova**, B.G. van Bloemen Waanders, S. Arunajatesan, M.F. Barone. "Stabilization of Projection-Based Reduced Order Models for Linear Time-Invariant Systems via Optimization-Based Eigenvalue Reassignment". *Comput. Meth. Appl. Mech. Engng.* **272** (2014) 251-270.

References (cont'd)

- Z. Wang, I. Akhtar, J. Borggaard, T. Iliescu. Proper orthogonal decomposition closure models for turbulent flows: a numerical comparison. *Comput. Methods Appl. Mech. Engrg.* **237-240**:10-26, 2012.
- **I. Kalashnikova**, S. Arunajatesan, M.F. Barone, B.G. van Bloemen Waanders, J.A. Fike. Reduced Order Modeling for Prediction and Control of Large-Scale Systems. *Sandia National Laboratories Report, SAND No. 2014-4693* (2014).
- **I. Kalashnikova**, S. Arunajatesan. A Stable Galerkin Reduced Order Model (ROM) for Compressible Flow, *WCCM-2012-18407*, *10th World Congress on Computational Mechanics (WCCM X),* Sao Paulo, Brazil (2012).
- K. Carlberg, C. Bou-Mosleh, C. Farhat. Efficient nonlinear model reduction via a least-squares Petrov-Galerkin projection and compressive tensor approximations. *Int. J. Numer. Meth. Engng.* **86** (2) 155-181 (2011).
- S. Chaturantabut, D.C. Sorensen. Discrete empirical interpolation for nonlinear model reduction. *Technical Report TR09-05*, Department of Computational and Applied Mathematics, Rice University (2009).
- **I. Kalashnikova**, B.G. van Bloemen Waanders, S. Arunajatesan, M.F. Barone. "Stabilization of Projection-Based Reduced Order Models for Linear Time-Invariant Systems via Optimization-Based Eigenvalue Reassignment". *Comput. Meth. Appl. Mech. Engng.* 272 (2014) 251-270.

Sandia National Laboratories

References (cont'd)

- The MathWorks, Inc., Optimization Toolbox User's Guide, 1990-2008.
- NICONET ROM benchmark repository: www.icm.tu-bs.de/NICONET/benchmodred.html.
- Oberwolfach ROM benchmark repository: http://simulation.uni-freiburg.de/downloads/benchmark.

Appendix: Stability Preserving ROM Approaches Literature Review

Approaches for building stability-preserving POD/Galerkin ROMs found in the literature fall into **two categories:**

Part 1 of talk.

1. ROMs which derive ***a priori*** a stability-preserving model reduction framework (usually specific to an equation set).

Can have an intrusive implementation

- ROMs based on projection in special ‘energy-based’ (not L^2) inner products, e.g., Rowley *et al*. (2004), Barone & Kalashnikova *et al.* (2009), Serre *et al*. (2012).

Part 2 of talk.

2. ROMs which stabilize an unstable ROM through an ***a posteriori*** post-processing stabilization step applied to the algebraic ROM system.

Can have inconsistencies between ROM and FOM physics

- Approaches in which an optimization problem that stabilizes an unstable ROM is formulated and solved, e.g., Amsallem *et al.* (2012), Bond *et al.* (2008), Kalashnikova *et al.* (2014).
- ROMs with increased numerical stability due to inclusion of ‘stabilizing’ terms in the ROM equations, e.g., Wang *et al.* (2012).

Appendix: Lyapunov Inner Product (Discrete Counterpart of Symmetry Inner Product)

Symmetry inner product has a discrete project counterpart!

- Consider a linear semi-discrete (i.e., discretized in space) stable FOM:

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{A}\boldsymbol{x}(t)$$

- The Lyapunov function for the above system is $V(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{P}\boldsymbol{x}$ where **P** is the solution of the following Ricatti equation:

$$\boldsymbol{A}^T\boldsymbol{P} + \boldsymbol{P}\boldsymbol{A} = -\boldsymbol{Q}$$

  - SPD solution to this Ricatti equation exists if $\boldsymbol{A}$ is stable and $\boldsymbol{Q}$ is SPD.
  - The solution to this Ricatti equation can be obtained using the MATLAB control toolbox:

```
P=lyap(A', Q, [], speye(n,n));
```

- Discrete analog of symmetry inner product: **Lyapunov inner product**

$$(\boldsymbol{x}_1, \boldsymbol{x}_2)_{\boldsymbol{P}} \equiv \boldsymbol{x}_1{}^T\boldsymbol{P}\boldsymbol{x}_2$$

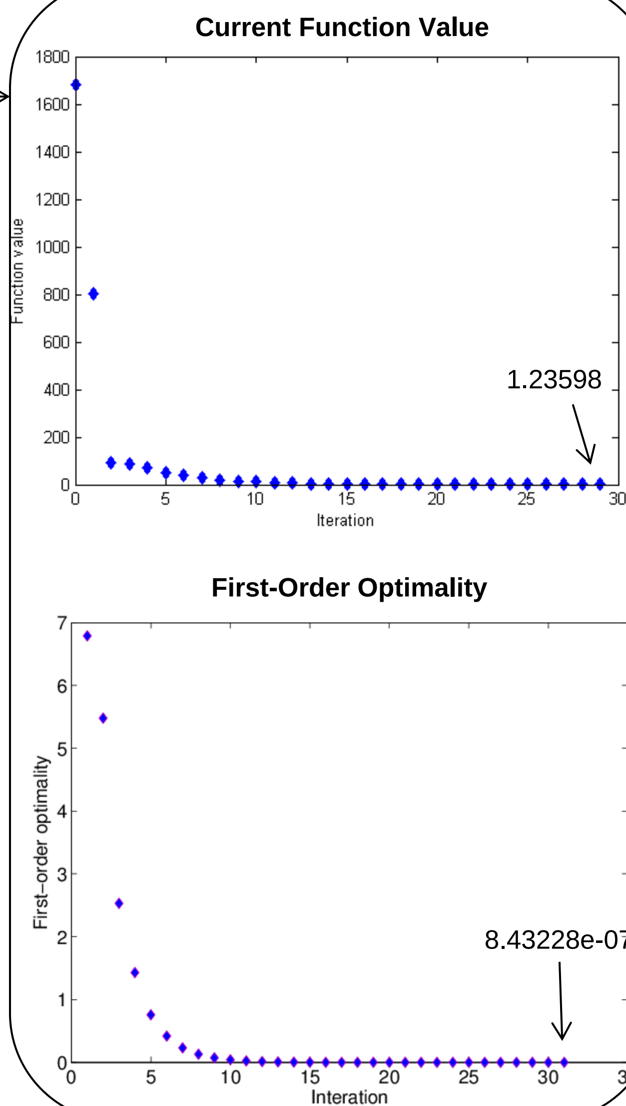
- Can show that if the ROM is constructed in the Lyapunov inner product, then:

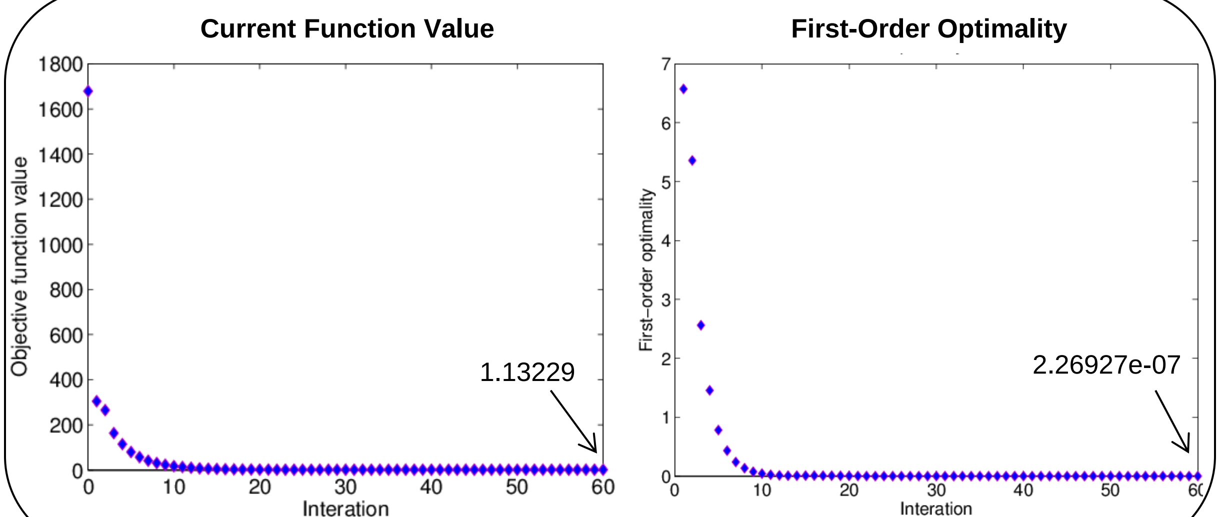
$$\frac{dE_M}{dt} \equiv \frac{1}{2}\frac{d}{dt}||\boldsymbol{x}_M||_2{}^2 \leq 0$$

Sandia National Laboratories

Appendix: Electrostatically Actuated Beam Benchmark (`fmincon` performance)

	Real Poles	Complex-Conjugate Poles
# upper bound constraints	4	2
# iterations	60	31
# function evaluations	64	32
$\lvert\nabla L\rvert$ at convergence (1st order optimality)	2.27e-7	8.43e-7





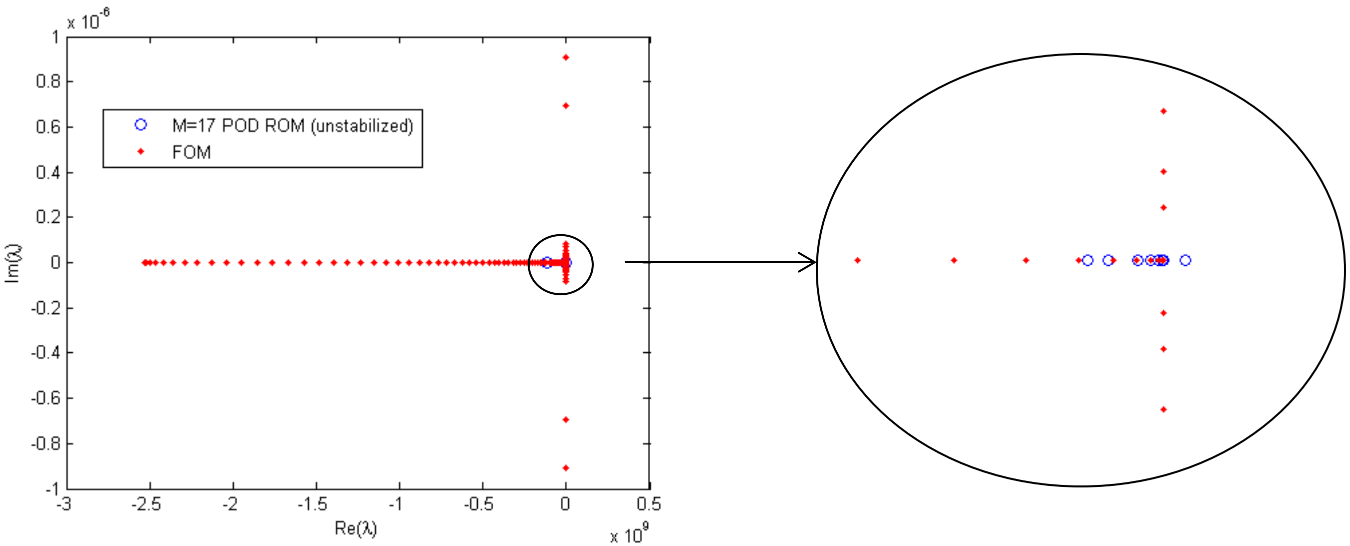
Appendix: Electrostatically Actuated Beam Benchmark (CPU Times)

Model	Operations	CPU time (sec)
FOM	Time-Integration	7.10e4
ROM – offline stage	Snapshot collection (FOM time-integration)	7.10e4
	Loading of matrices/snapshots	5.17
	POD	1.09e1
	Projection	2.55e1
	Optimization	8.79e1
ROM – online stage	Time-integration	6.78

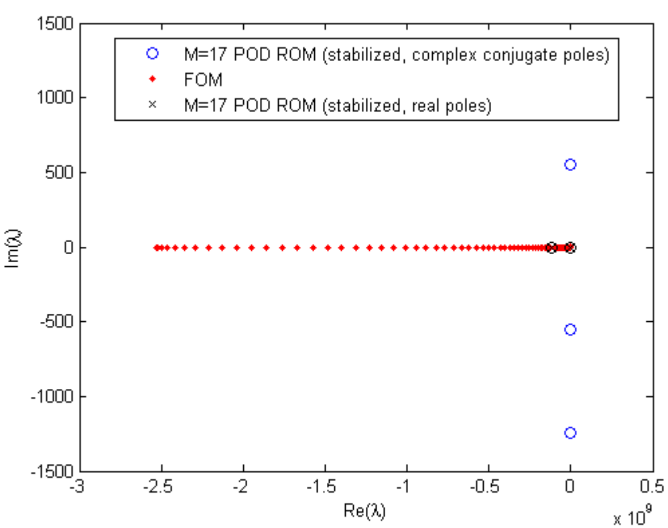
- To offset total pre-process time of ROM (time required to run FOM to collect snapshots, calculate the POD basis, perform the Galerkin projection, and solve the optimization problem (1)), the ROM would need to be run 1e4 times (due to large CPU time of FOM).
- Solution of optimization problem is very fast: takes ~1.5 minute to complete.

Sandia National Laboratories

Appendix: Electrostatically Actuated Beam Benchmark (Eigenvalues)



Unstable Eigenvalues
$\lambda_6 = 16{,}053$
$\lambda_{12} = 48.985$
$\lambda_{14} = 12.650$
$\lambda_{17} = 0.05202$



Stabilized Eigenvalues (Real)	Stabilized Eigenvalues (Complex Conjugates)
$\lambda_6 = -7{,}043{,}505$	$\lambda_6 = -106{,}976 + 551.77i$
$\lambda_{12} = -35.364$	$\lambda_{12} = -106{,}976 - 551.77$
$\lambda_{14} = -153{,}033$	$\lambda_{14} = -2954.1 - 1244.7i$
$\lambda_{17} = -99{,}175$	$\lambda_{17} = -2954.1 + 1244.7i$